

# SELF-ADJOINT, GLOBALLY DEFINED HAMILTONIAN OPERATORS FOR SYSTEMS WITH BOUNDARIES

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ABSTRACT. For a general self-adjoint Hamiltonian operator  $H_0$  on the Hilbert space  $L^2(\mathbb{R}^d)$ , we determine the set of all self-adjoint Hamiltonians  $H$  on  $L^2(\mathbb{R}^d)$  that dynamically confine the system to an open set  $\Omega \subset \mathbb{R}^d$  while reproducing the action of  $H_0$  on an appropriate operator domain. In the case  $H_0 = -\Delta + V$  we construct these Hamiltonians explicitly showing that they can be written in the form  $H = H_0 + B$ , where  $B$  is a singular boundary potential and  $H$  is self-adjoint on its maximal domain.

## 1. INTRODUCTION.

This paper concerns the quantum formulation of systems with boundaries. These systems play an important part in several fields of current research like, for instance, in mathematical physics (e.g. the theory of self-adjoint extensions of symmetric operators [35, 28, 29, 18, 42, 1, 34, 6, 46, 38, 9, 45, 20, 40, 8, 15]), condensed matter physics (e.g. the quantum description of particles moving on surfaces with obstacles or impurities [30, 12]) and in string theory [47, 37] and other modern approaches to quantum gravity [26, 19] (where the classical theory displays a non-trivial global structure [26]).

Let us consider a  $d$ -dimensional dynamical system confined to an open set  $\Omega \subset \mathbb{R}^d$ . Two main approaches to the canonical quantization of these systems [20], are:

(A) The kinematical approach, where the confinement is a consequence of the choice of the Hilbert space, assumed to be  $L^2(\Omega)$ .

(B) The dynamical approach, where the system is formulated in the unconfined Hilbert space  $L^2(\mathbb{R}^d)$  and the confinement is a feature of dynamics i.e. it is a consequence of the choice of the Hamiltonian operator.

In both cases one is faced with the problem of determining self-adjoint (s.a.) realizations of the Hamiltonian operator (i.e. to determine a formal s.a. differential expression and a domain such that  $H = H^*$ ). Notice that the implementation of the Hamiltonian operator (as well as other fundamental observables) only as a symmetric operator ( $S \subset S^*$ ) does not provide a suitable definition of a physical observable (see e.g. [36]). The difference between symmetric and s.a. operators is an important one but also a subtle one, that can only be seen from the analysis of the operator domains. One of the aims of this paper is precisely to show that, through the approach (B), the symmetric Hamiltonian, its adjoint and each of its s.a. realizations can be naturally defined by a particular differential expression.

A more detailed analysis shows that, at a fundamental level the (more standard) approach (A) reveals unexpected inconsistencies [20, 9, 26]. These are mainly related to ambiguities in the physical predictions (when there are several possible self-adjoint realizations of a single observable) or to the absence of self-adjoint (s.a.) formulations of important observables. These difficulties are well illustrated by the textbook example of a one-dimensional single particle described by the Hamiltonian  $H = -\frac{d^2}{dx^2}$ , and confined to the positive half-line [1, 20].

The approach (B), on the other hand, displays the obvious advantage that the most important observables (like the momentum) are naturally defined as s.a. operators. The main problem is the construction of s.a. Hamiltonians defined on  $L^2(\mathbb{R}^d)$  but effectively confining the system to its domain  $\Omega \subset \mathbb{R}^d$ . This approach has been scarcely explored in the literature. Up to our knowledge, one of the few references in the subject is [20] where the authors propose and study some of the features of a mechanism for dynamical confinement. Some related work on the relations between partially and globally defined operators was presented in [45].

In this paper we shall further study the dynamical confinement point of view. The problems that will be addressed are closely related to the topics of singular perturbations of s.a. operators [2, 38], point interaction Hamiltonians [2, 4, 7] and s.a. extensions of symmetric restrictions [20, 40]. Our starting point will be a generic unconfined dynamical system defined on the Hilbert space  $L^2(\mathbb{R}^d)$  and described by a s.a. Hamiltonian  $H_0$ .

Given an open set  $\Omega \subset \mathbb{R}^d$  and denoting by  $\chi_\Omega$  its characteristic function, we consider the orthogonal projection

$$P_\Omega : L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d), \quad P_\Omega \psi = \chi_\Omega \psi,$$

so that

$$L^2(\mathbb{R}^d) \simeq \text{Ran}(P_\Omega) \oplus \text{Ker}(P_\Omega) \equiv L^2(\Omega) \oplus L^2(\Omega^c).$$

This paper is devoted to solving the two following problems:

**Problem 1.** *Given a s.a. linear operator*

$$H_0 : D(H_0) \subseteq L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d),$$

*determine the explicit form of all linear operators*

$$H : D(H) \subseteq L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d)$$

*that satisfy the following three properties:*

- (1)  $P_\Omega(D(H)) \subseteq D(H)$  and  $[P_\Omega, H]\psi = 0$  for all  $\psi \in D(H)$ ;
- (2)  $H$  is self-adjoint;
- (3) if  $\psi \in D(H_0)$  is an eigenstate of  $P_\Omega$  then  $\psi \in D(H)$  and  $H\psi = H_0\psi$ .

We will refer to the operators  $H$  as the *confining Hamiltonians* and to the properties (1) to (3) as the *defining properties of  $H$* .

From (1) and (2) we find that  $P_\Omega$  commutes with all the spectral projectors of  $H$  and so also with the operator  $e^{-itH}$ . Hence, if  $\psi$  is an eigenstate of  $P_\Omega$  (with eigenvalue 0 or 1) it will evolve to  $e^{-itH}\psi$ , which is again an eigenstate of  $P_\Omega$  with the same eigenvalue. In other words,  $P_\Omega$  is a constant of the motion and a wave function confined to  $\Omega$  (or to  $\Omega^c$ ) will stay so forever. Finally, property (3) imposes that, within the subspace  $L^2(\Omega)$  (or  $L^2(\Omega^c)$ ), the time evolution determined by  $H$  reproduces the original one given by  $H_0$ .

**Problem 2.** *For  $H_0 = -\Delta + V$  determine whether it is possible to write the corresponding confining Hamiltonians  $H$  (solutions of Problem 1) in the form  $H = H_0 + B$  where  $B$  is a singular boundary potential and  $H$  is s.a. on its maximal domain.*

The first part of this paper (section 2) is devoted to Problem 1. We shall characterize the operators that satisfy properties (1) to (3), determine the properties that the original  $H_0$  should satisfy so that the operators  $H$  do exist and derive a method to construct these operators explicitly. In this context we will also explore the relations between partially and globally defined operators. The results of this section lead naturally to the construction of yet another class of s.a. Hamiltonians, which describe systems composed of separate domains but allow for some sort of information transfer between these domains. Further investigation on these operators will be left for a future work [17].

The second part of the paper (section 3) is devoted to Problem 2. We specialize to Hamiltonians of the form  $H_0 = -\Delta + V$  and introduce a new kind of singular operators. These will be used to write the Hamiltonians  $H$ , satisfying the three defining properties, in the desired form:  $H = H_0 + B$ , where  $B$  is a singular boundary potential which is dependent of the boundary conditions that characterize the domain of  $H$ . This is always possible. Indeed  $H$  amounts to a self-adjoint extension of the symmetric restriction of  $H_0$  to the domain  $D(\Delta_{\Omega_1}^{\min}) \oplus D(\Delta_{\Omega_2}^{\min})$ , where  $\Delta_{\Omega_k}^{\min}$ ,  $k = 1, 2$ , denotes the minimal Laplacian on  $\Omega_k$  with operator domain given by the set of smooth functions with compact support contained in  $\Omega_k$ ,  $\Omega_1 = \Omega$ ,  $\Omega_2 = (\bar{\Omega})^c$ . Thus, by the additive representation of self-adjoint extensions obtained in [39] (also see [40]),  $H$  admits the additive representation  $H = -\Delta + V + B$ , where  $B$  is a singular boundary potential which we explicitly determine. Such a singular boundary potential is defined in terms of the zero'th and first order trace operators on the boundary or better of their extensions (provided in [31, 32]) to the maximal domains  $D(\Delta_{\Omega_k}^{\max}) = \{\psi_k \in L^2(\Omega_k) : \Delta_{\Omega_k} \psi_k \in L^2(\Omega_k)\}$ .

As final result of the paper, we show that the operators  $H$  are s.a. on their maximal domain. Hence, contrary to what is common in the approach (A), there is no ambiguity regarding the boundary conditions satisfied by the domain of  $H$ . In fact, each  $H$  satisfying (1) to (3) exhibits a particular functional form  $H = H_0 + B$  (it displays a particular boundary potential  $B$ ) and its self-adjointness domain turns out to be its maximal domain.

Finally, let us point out that there are some interesting topics related to the results of this paper that could be studied. These may include: the global formulation of systems composed by several domains and displaying some kind of information transfer between different domains; the application of the results of this paper to the deformation quantization of confined systems [3, 27, 16] and to the noncommutative formulation of manifolds with boundaries [14, 33].

## 2. CONFINING HAMILTONIANS ON $L^2(\mathbb{R}^d)$

In this section we will study the operators

$$H : D(H) \subseteq L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d)$$

associated to a s.a.  $H_0$ , and satisfying the defining properties (1) to (3). We will prove that all these operators are of the form  $H = H_1 \oplus H_2$  where  $H_1$  and  $H_2$  are s.a extensions of the restrictions of  $H_0$  to a suitable domain.

Given the open set  $\Omega \subset \mathbb{R}^d$ , we pose

$$\Omega_1 := \Omega, \quad \Omega_2 := (\bar{\Omega}_1)^c$$

and use the decomposition of the orthogonal projection

$$P_k \equiv P_{\Omega_k} = E_k R_k, \quad E_k = R_k^*, \quad k = 1, 2,$$

given by the restriction and extension operators

$$R_k : L^2(\mathbb{R}^d) \rightarrow L^2(\Omega_k), \quad [R_k \psi](x) := \psi(x), \quad x \in \Omega_k,$$

$$E_k : L^2(\Omega_k) \rightarrow L^2(\mathbb{R}^d), \quad [E_k \psi_k](x) := \begin{cases} \psi_k(x) & x \in \Omega_k \\ 0 & x \in \Omega_k^c. \end{cases}$$

By such operators one has the identification

$$L^2(\Omega_1) \oplus L^2(\Omega_2) \simeq L^2(\mathbb{R}^d)$$

given by the unitary map

$$J : L^2(\Omega_1) \oplus L^2(\Omega_2) \rightarrow L^2(\mathbb{R}^d), \quad J(\psi_1 \oplus \psi_2) := E_1 \psi_1 + E_2 \psi_2,$$

with inverse

$$J^{-1} : L^2(\mathbb{R}^d) \rightarrow L^2(\Omega_1) \oplus L^2(\Omega_2), \quad J^{-1} \psi := R_1 \psi \oplus R_2 \psi.$$

Given two linear operators

$$L_k : D(L_k) \subseteq L^2(\Omega_k) \rightarrow L^2(\Omega_k), \quad k = 1, 2$$

we pose as usual

$$L_1 \oplus L_2 : D(L_1) \oplus D(L_2) \subseteq L^2(\Omega_1) \oplus L^2(\Omega_2) \rightarrow L^2(\Omega_1) \oplus L^2(\Omega_2),$$

$$L_1 \oplus L_2 \psi_1 \oplus \psi_2 := L_1 \psi_1 \oplus L_2 \psi_2.$$

Given any two subspaces  $V_k \subseteq L^2(\Omega_k)$ , we define the subspace  $V_1 \tilde{\oplus} V_2 \subseteq L^2(\mathbb{R}^d)$  by

$$V_1 \tilde{\oplus} V_2 := J(V_1 \oplus V_2),$$

and then the operator on  $L^2(\mathbb{R}^d)$

$$L_1 \tilde{\oplus} L_2 : D(L_1) \tilde{\oplus} D(L_2) \subseteq L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d),$$

$$L_1 \tilde{\oplus} L_2 := J(L_1 \oplus L_2) J^{-1}.$$

Then one has the following

**Theorem 2.1.** *A linear operator  $H : D(H) \subseteq L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d)$  satisfies the defining property (1) above iff it can be written in the form*

$$H = H_1 \tilde{\oplus} H_2 : D(H_1) \tilde{\oplus} D(H_2) \subseteq L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d),$$

where

$$H_k : D(H_k) := R_k(D(H)) \subseteq L^2(\Omega_k) \rightarrow L^2(\Omega_k), \quad H_k := R_k H E_k.$$

*Proof.* By known results on reducing subspaces (see e.g. [6], Chapter 3, Section 6) one has that property (1) holds true iff  $L^2(\Omega)$  reduces  $H$ . Thus

$$HP_k(D(H)) \subseteq P_k(L^2(\mathbb{R}^d))$$

and

$$H\psi = P_1HP_1\psi + P_2HP_2\psi.$$

Hence

$$\begin{aligned} H\psi &= E_1R_1HE_1R_1\psi + E_2R_2HE_2R_2\psi \\ &= J(R_1HE_1R_1\psi + R_2HE_2R_2\psi) \\ &= J(R_1HE_1 \oplus R_2HE_2)J^{-1}\psi. \end{aligned}$$

□

**Remark 2.2.** By the known properties of direct sums of operators, and since  $H_1 \oplus H_2$  and  $H_1 \tilde{\oplus} H_2$  are unitarily equivalent, one has that

$$H \text{ is symmetric iff } H_1 \text{ and } H_2 \text{ are symmetric,}$$

and, in the case both  $D(H_1)$  and  $D(H_2)$  are dense,

$$H^* = H_1^* \tilde{\oplus} H_2^*.$$

Be aware that here and below by symmetric operator we just mean a linear operator  $S$  such that  $\langle S\phi, \psi \rangle = \langle \phi, S\psi \rangle$  for all  $\phi, \psi \in D(S)$ ; the operator domain  $D(S)$  could be not dense.

In particular  $H$  is self-adjoint iff  $H_1$  and  $H_2$  are both self-adjoint. Thus a Hamiltonian  $H$  satisfies the defining properties (1) and (2) iff it can be written in the form  $H = H_1 \tilde{\oplus} H_2$  where  $H_1$  and  $H_2$  are given in the previous theorem and self-adjoint.

We now investigate the implications of the defining property (3).

Let us consider the operators

$$S_k : D(S_k) \subseteq L^2(\Omega_k) \rightarrow L^2(\Omega_k), \quad S_k := R_k H_0 E_k$$

$$D(S_k) := \{\psi_k \in L^2(\Omega_k) : E_k \psi_k \in D(H_0)\}.$$

For any  $\phi_k, \psi_k \in D(S_k)$  one has

$$\begin{aligned} \langle R_k H_0 E_k \phi_k, \psi_k \rangle_{L^2(\Omega_k)} &= \langle H_0 E_k \phi_k, E_k \psi_k \rangle_{L^2(\mathbb{R}^d)} \\ &= \langle E_k \phi_k, H_0 E_k \psi_k \rangle_{L^2(\mathbb{R}^d)} = \langle \phi_k, R_k H_0 E_k \psi_k \rangle_{L^2(\Omega_k)} \end{aligned}$$

and so  $S_k$  is a symmetric operator. Then is immediate to check that property (3) is equivalent to

$$\tilde{H}_0 \subseteq H,$$

where  $\tilde{H}_0$  denotes the symmetric operator given by the restriction of  $H_0$  to  $D(S_1) \tilde{\oplus} D(S_2)$ . Thus (1) puts the constraint

$$(2.1) \quad [P_\Omega, \tilde{H}_0] = 0$$

on  $H_0$ . By (2.1) and Theorem 2.1 one gets

$$\tilde{H}_0 = S_1 \tilde{\oplus} S_2$$

and so

**Theorem 2.3.** *Let  $H_0$  be a s.a. operator. If  $[P_\Omega, \tilde{H}_0] \neq 0$  then there is no operator  $H$  satisfying (1) to (3). If, on the other hand,  $[P_\Omega, \tilde{H}_0] = 0$  then  $H$  satisfies (1) to (3) if and only if the symmetric operators  $S_k$  admit self-adjoint extensions  $H_k$  and  $H = H_1 \tilde{\oplus} H_2$ .*

**Remark 2.4.** Let us suppose that both the domains of the symmetric operators  $S_1$  and  $S_2$  are dense. From Remark 2.2 we know that the adjoint of  $S_1 \tilde{\oplus} S_2$  is  $S_1^* \tilde{\oplus} S_2^*$  and so the operators  $H$  are s.a. restrictions of  $S_1^* \tilde{\oplus} S_2^*$  of the kind  $H_1 \tilde{\oplus} H_2$ . An interesting point is the relation between the s.a. extensions of  $S_1$ ,  $S_2$  and the s.a. extensions of  $S_1 \tilde{\oplus} S_2$ . To characterize the s.a. extensions of  $S_1 \tilde{\oplus} S_2$  we need the deficiency subspaces  $N_\pm^{1,2}$  of  $S_1 \oplus S_2$ . Since

$$\begin{aligned} N_\pm^{1,2} &= \{\psi_1 \oplus \psi_2 \in D(S_1^*) \oplus D(S_2^*) : S_1^* \oplus S_2^* (\psi_1 \oplus \psi_2) = \pm i \psi_1 \oplus \psi_2\} \\ &= N_\pm^1 \oplus N_\pm^2 \end{aligned}$$

where  $N_\pm^1$  and  $N_\pm^2$  are the deficiency subspaces of  $S_1$  and  $S_2$  respectively. If  $d = 1$  then the deficiency subspaces are finite dimensional and the deficiency indices satisfy

$$m_\pm = \dim N_\pm^{1,2} = \dim N_\pm^1 + \dim N_\pm^2 = m_\pm^1 + m_\pm^2.$$

We immediately notice that  $S_1$  and  $S_2$  may have no s.a. extensions (because  $m_-^1 \neq m_+^1$  and  $m_-^2 \neq m_+^2$ ) and yet  $S_1 \oplus S_2$  may have s.a. extensions (which will not be of the form  $H_1 \oplus H_2$ ). In the case  $d > 1$  the situation is similar. Here the deficiency subspaces  $N_\pm^1$  and  $N_\pm^2$  are infinite dimensional and  $S_1$  and  $S_2$  have non-self-adjoint maximal extension (see e.g. [8], Theorem 4.7.9) which however could produce self-adjoint extensions of  $S_1 \oplus S_2$ .

We already know from Remark 2.2 that if  $H_1$  and  $H_2$  are s.a. extensions of  $S_1$  and  $S_2$  then  $H_1 \oplus H_2$  is a s.a. extension of  $S_1 \tilde{\oplus} S_2$ . However, the converse result is not valid, i.e. not all s.a. extensions of  $S_1 \oplus S_2$  are of the form  $H_1 \oplus H_2$  with  $H_1$  and  $H_2$  self-adjoint. Indeed according to von Neumann's theorem [35, 1], the s.a. extensions of  $S_1 \tilde{\oplus} S_2$  are parametrized by the unitary operators  $U : N_+^{1,2} \rightarrow N_-^{1,2}$  while the ones of  $S_k$  are parametrized by the unitary operators  $U_k : N_+^k \rightarrow N_-^k$ . Since

there are lots of unitary operators  $U : N_+^1 \oplus N_+^2 \rightarrow N_-^1 \oplus N_-^2$  which are not of the form  $U_1 \oplus U_2$ , there are lots of extensions of  $S_1 \oplus S_2$  which are not of the form  $H_1 \oplus H_2$ . It follows from Theorem 2.3 that these are not confining. We shall designate them by *transversal*, because they are associated with boundary conditions relating the wave functions of the two domains.

### 3. BOUNDARY POTENTIALS

Let us now suppose that  $H_0$  is given by the Schrödinger operator  $H_0 = -\Delta + V$ . We take  $V \in L^\infty(\mathbb{R}^d)$  so that it induces a bounded multiplication operator and  $H_0$  is self-adjoint with domain  $D(H_0) = H^2(\mathbb{R}^d)$ . Here  $H^2(\mathbb{R}^d)$ , the self-adjointness domain of  $-\Delta$ , denotes the Sobolev-Hilbert space, with scalar product

$$\langle \phi, \varphi \rangle_{H^2(\mathbb{R}^d)} := \langle \Delta \phi, \Delta \varphi \rangle_{L^2(\mathbb{R}^d)} + \langle \phi, \varphi \rangle_{L^2(\mathbb{R}^d)},$$

of square-integrable functions with square integrable distributional Laplacian. Thus  $H^2(\mathbb{R}^d)$  coincides with the maximal domain of definition of  $H_0$ . Then we suppose that  $\Omega \subset \mathbb{R}^d$  is an open bounded set with a boundary  $\Gamma$  which is a smooth embedded  $(d-1)$ -dimensional manifold.

**Remark 3.1.** Both our hypotheses on the potential  $V$  and the boundary  $\Gamma$  could be weakened. We take here the simplest ones in order to avoid too many technicalities. Regarding the potential we could require that it is relatively  $-\Delta$ -bounded with bound  $< 1$ , so that, by the Kato-Rellich theorem,  $H_0$  is still self-adjoint with domain  $H^2(\mathbb{R}^d)$ . Regarding the boundary  $\Gamma$  everything continues to hold (with the same proofs) with  $\Gamma$  of class  $C^{1,1}$ , i.e.  $\Gamma$  is locally the graph of a  $C^1$  function with Lipschitz derivatives. With some more work  $\Omega$  could be supposed to have no more than a Lipschitz boundary, the minimal requirement in order to define (almost everywhere on  $\Gamma$ ) the normal at the boundary.

As in the previous section we pose

$$\Omega_1 := \Omega, \quad \Omega_2 := (\bar{\Omega}_1)^c$$

and we denote by  $H^n(\Omega_k)$ ,  $k = 1, 2$ ,  $n$  a positive integer, the Sobolev-Hilbert space given by completing the pre-Hilbert space  $R_k(C_c^\infty(\mathbb{R}^d))$  endowed with the scalar product

$$\langle \phi, \varphi \rangle_{H^n(\Omega_k)} = \sum_{0 \leq \alpha_1 + \dots + \alpha_d \leq n} \langle \partial_{x_1}^{\alpha_1} \dots \partial_{x_d}^{\alpha_d} \phi, \partial_{x_1}^{\alpha_1} \dots \partial_{x_d}^{\alpha_d} \varphi \rangle_{L^2(\Omega_k)}.$$

Analogously  $H_0^n(\Omega_k) \subsetneq H^n(\Omega_k)$  denotes the completion of pre-Hilbert space  $C_c^\infty(\Omega_k)$  endowed with the same scalar product as  $R_k(C_c^\infty(\mathbb{R}^d))$ .



Obviously the extension operator

$$E_k : C_c^\infty(\Omega_k) \rightarrow C_c^\infty(\mathbb{R}^d)$$

is continuous with respect to the  $H^2$ -type norms. Since  $C_c^\infty(\Omega_k)$  and  $C_c^\infty(\mathbb{R}^d)$  are dense in  $H_0^2(\Omega_k)$  and  $H^2(\mathbb{R}^d)$  respectively,

$$E_k : H_0^2(\Omega_k) \rightarrow H^2(\mathbb{R}^d)$$

and

$$S_k : H_0^2(\Omega_k) \subset L^2(\Omega_k) \rightarrow L^2(\Omega_k), \quad S_k = R_k H_0 E_k = -\Delta_{\Omega_k} + V_k$$

is a well-defined densely defined closed symmetric operator. Here  $\Delta_{\Omega_k}$  denotes the distributional Laplacian on  $L^2(\Omega_k)$  and  $V_k := R_k V E_k$ . Moreover  $S_k$  has self-adjoint extensions and all such extensions can be explicitly characterized in terms of (eventually non-local) boundary conditions (see [24, 40, 41, 25] and references therein, the study of boundary value problems by means of self-adjoint extensions goes back to [13] and was further developed in [44]; for other recent results see [5], [43], [10], [21], [22], [11]).

Thus, since  $H_0 = -\Delta + V$  satisfies (2.1), according to Theorem 2.3 any  $H$  of the kind  $H = H_1 \tilde{\oplus} H_2$ , where  $H_k$  is a self-adjoint extension of  $S_k$ , satisfies properties (1) to (3).

We want now to recast the above operator  $H$  in the form

$$H = -\Delta + V + B,$$

where  $B$  is some singular boundary potential supported on  $\Gamma$ . This is always possible. Indeed  $H$  is a self-adjoint extension of the symmetric operator  $S_1 \tilde{\oplus} S_2$  given by restricting the self-adjoint operator  $H_0$  to the dense domain  $H_0^2(\Omega_1) \tilde{\oplus} H_0^2(\Omega_2)$ . By [39] any self-adjoint extension of a symmetric restriction of  $H_0$  admits the additive representation  $H = -\Delta + V + B$ , where  $B$  is some singular boundary operator. Such operator  $B$  could be obtained by using the general theory developed in [39], but for the case here considered we prefer to present a more explicit (although equivalent) construction.

We know that the self-adjoint  $H$  is the restriction of  $S_1^* \tilde{\oplus} S_2^*$  to  $D(H_1) \tilde{\oplus} D(H_2)$ , where  $S_k^*$  is explicitly given by (see e.g. [24, 40, 41])

$$S_k^* : D(\Delta_{\Omega_k}^{\max}) \subseteq L^2(\Omega_k) \rightarrow L^2(\Omega_k), \quad S_k^* \psi_k := -\Delta_{\Omega_k} \psi_k + V_k \psi_k,$$

$$D(\Delta_{\Omega_k}^{\max}) := \{\psi_k \in L^2(\Omega_k) : \Delta_{\Omega_k} \psi_k \in L^2(\Omega_k)\}.$$

It is known that  $D(\Delta_{\Omega_k}^{\max}) = H^2(\Omega_k)$  if  $d = 1$ , otherwise  $H^2(\Omega_k)$  is strictly contained in  $D(\Delta_{\Omega_k}^{\max})$ .

From now on we will use the notation  $\mathscr{D}'(M)$  for the space of distributions on the set  $M$  with corresponding test function space  $\mathscr{D}(M) \equiv C_c^\infty(M)$ ;  $\langle \cdot, \cdot \rangle$  will denote the  $\mathscr{D}'(M)$ - $\mathscr{D}(M)$  pairing.

Let

$$\psi = \chi_{\Omega_1}\phi_1 + \chi_{\Omega_2}\phi_2 \equiv J(R_1\phi_1 \oplus R_2\phi_2), \quad \phi_k \in \mathcal{D}(\mathbb{R}^d).$$

Then  $\psi \in D(\Delta_{\Omega_1}^{\max}) \tilde{\oplus} D(\Delta_{\Omega_2}^{\max})$  and

$$S_1^* \tilde{\oplus} S_2^* \psi = -\chi_{\Omega_1}\Delta\phi_1 - \chi_{\Omega_2}\Delta\phi_2 + V\psi.$$

By the distributional Leibniz rule,

$$\Delta(\chi_{\Omega_k}\phi) = \phi\Delta\chi_{\Omega_k} + 2\nabla\chi_{\Omega_k} \cdot \nabla\phi + \chi_{\Omega_k}\Delta\phi.$$

By the Gauss-Green formula one has, for any test function  $\varphi \in \mathcal{D}(\mathbb{R}^d)$ ,

$$\langle \nabla\chi_{\Omega_k}, \varphi \rangle = - \int_{\Omega_k} \nabla\varphi(x) dx = - \int_{\Gamma} n_k(x)\varphi(x) d\sigma_{\Gamma}(x),$$

where  $n_k$  denotes the outer (w.r.t.  $\Omega_k$ ) normal at  $\Gamma$  and  $\sigma_{\Gamma}$  is the surface measure of  $\Gamma$ . Given the continuous linear map

$$\rho : \mathcal{D}(\mathbb{R}^d) \rightarrow \mathcal{D}(\Gamma), \quad [\rho\varphi](x) := \varphi(x), \quad x \in \Gamma,$$

we define  $\delta_{\Gamma} \in \mathcal{D}'(\mathbb{R}^d)$  by

$$\delta_{\Gamma} : \mathcal{D}(\mathbb{R}^d) \rightarrow \mathbb{C}, \quad \langle \delta_{\Gamma}, \varphi \rangle := \langle 1, \rho\varphi \rangle \equiv \int_{\Gamma} \varphi(x) d\sigma_{\Gamma}(x),$$

and  $f\delta_{\Gamma} \in \mathcal{D}'(\mathbb{R}^d)$ ,  $f \in \mathcal{D}'(\Gamma)$ , by

$$f\delta_{\Gamma} : \mathcal{D}(\mathbb{R}^d) \rightarrow \mathbb{C}, \quad \langle f\delta_{\Gamma}, \varphi \rangle := \langle f, \rho\varphi \rangle.$$

Then

$$\nabla\chi_{\Omega_k} = -n_k \delta_{\Gamma}, \quad \Delta\chi_{\Omega_k} = \nabla \cdot \nabla\chi_{\Omega_k} = -\nabla \cdot (n_k \delta_{\Gamma}).$$

and so, for any  $\psi = \chi_{\Omega_1}\phi_1 + \chi_{\Omega_2}\phi_2$ ,  $\phi_k \in \mathcal{D}(\mathbb{R}^d)$ , since

$$n \equiv n_1 = -n_2,$$

one has

$$\begin{aligned} S_1^* \tilde{\oplus} S_2^* \psi &= -\Delta\psi + V\psi + (\Delta\psi - \chi_{\Omega_1}\Delta\phi_1 - \chi_{\Omega_2}\Delta\phi_2) \\ &= -\Delta\psi + V\psi - 2(\nabla(\phi_1 - \phi_2)) \cdot n \delta_{\Gamma} - (\phi_1 - \phi_2) \nabla(n \cdot \delta_{\Gamma}). \end{aligned}$$

Now we introduce

$$\gamma_{\Omega_k}^0 : H^2(\Omega_k) \rightarrow L^2(\Gamma), \quad \gamma_{\Omega_k}^1 : H^2(\Omega_k) \rightarrow L^2(\Gamma)$$

defined as the unique continuous linear maps such that, when  $\psi_k = R_k\phi_k$ ,  $\phi_k \in \mathcal{D}(\mathbb{R}^d)$ ,

$$[\gamma_{\Omega_k}^0 \psi_k](x) = \phi_k(x), \quad [\gamma_{\Omega_k}^1 \psi_k](x) = n_k(x) \cdot \nabla\phi_k(x), \quad x \in \Gamma.$$

More precisely these trace operators have range respectively given by the fractional Sobolev spaces  $H^{3/2}(\Gamma)$  and  $H^{1/2}(\Gamma)$  (see e.g. [32], Chapter 1, Section 8.2). These maps have unique continuous extensions (see [31], Sections 2 and 3, [32], Chapter 2, Section 6.5)

$$\hat{\gamma}_{\Omega_k}^0 : D(\Delta_{\Omega_k}^{\max}) \rightarrow \mathcal{D}'(\Gamma), \quad \hat{\gamma}_{\Omega_k}^1 : D(\Delta_{\Omega_k}^{\max}) \rightarrow \mathcal{D}'(\Gamma).$$

More precisely these maps have range respectively given by the dual Sobolev spaces  $H^{-1/2}(\Gamma)$  and  $H^{-3/2}(\Gamma)$ . Let us remark that the results we need here and below from the quoted references [31, 32] were proved there in the case of a bounded set, an hypothesis which  $\Omega^c$  does not satisfy; however what really counts is not the boundedness of  $\Omega^c$  but the compactness of its boundary: one can check that this alternative hypothesis suffices (see e.g. [25]).

One has

$$H_0^2(\Omega_k) = \{\psi_k \in H^2(\Omega_k) : \gamma_k^0 \psi_k = \gamma_k^1 \psi_k = 0\}$$

and, by elliptic regularity (see [32], Chapter 2, Section 7.3),

$$(3.1) \quad H^2(\Omega_k) = \{\psi_k \in D(\Delta_{\Omega_k}^{\max}) : \hat{\gamma}_{\Omega_k}^0 \psi_k \in H^{3/2}(\Gamma)\}$$

$$(3.2) \quad = \{\psi_k \in D(\Delta_{\Omega_k}^{\max}) : \hat{\gamma}_{\Omega_k}^1 \psi_k - f_k \hat{\gamma}_{\Omega_k}^0 \psi_k \in H^{1/2}(\Gamma)\},$$

where  $f_k \in C^\infty(\Gamma)$ .

By  $\hat{\gamma}_{\Omega_k}^0$  and  $\hat{\gamma}_{\Omega_k}^1$  we can then define the continuous linear maps

$$j_\Gamma^0 : D(\Delta_{\Omega_1}^{\max}) \tilde{\oplus} D(\Delta_{\Omega_2}^{\max}) \rightarrow \mathcal{D}'(\Gamma), \quad j_\Gamma^0 \psi := \hat{\gamma}_{\Omega_1}^0 \psi_1 - \hat{\gamma}_{\Omega_2}^0 \psi_2,$$

$$j_\Gamma^1 : D(\Delta_{\Omega_1}^{\max}) \tilde{\oplus} D(\Delta_{\Omega_2}^{\max}) \rightarrow \mathcal{D}'(\Gamma), \quad j_\Gamma^1 \psi := \hat{\gamma}_{\Omega_1}^1 \psi_1 + \hat{\gamma}_{\Omega_2}^1 \psi_2,$$

which measure the jumps of  $\psi = E_1 \psi_1 + E_2 \psi_2$  and of its normal derivative across  $\Gamma$ . Thus, for any  $\psi = \chi_{\Omega_1} \phi_1 + \chi_{\Omega_2} \phi_2$ ,  $\phi_k \in \mathcal{D}(\mathbb{R}^d)$ , since

$$\begin{aligned} \langle (\nabla(\phi_1 - \phi_2)) \cdot n \delta_\Gamma, \varphi \rangle &= \langle n \cdot \delta_\Gamma, \varphi \nabla(\phi_1 - \phi_2) \rangle \\ &= \int_\Gamma \varphi(x) n(x) \cdot \nabla(\phi_1 - \phi_2)(x) d\sigma_\Gamma(x) = \langle j_\Gamma^1 \psi \delta_\Gamma, \varphi \rangle \end{aligned}$$

and

$$\begin{aligned}
& \langle (\phi_1 - \phi_2) \nabla \cdot (n \delta_\Gamma), \varphi \rangle = \langle \nabla \cdot (n \delta_\Gamma), \varphi(\phi_1 - \phi_2) \rangle \\
& = - \int_\Gamma n(x) \cdot \nabla (\varphi(\phi_1 - \phi_2))(x) d\sigma_\Gamma(x) \\
& = - \int_\Gamma (\phi_1 - \phi_2)(x) n(x) \cdot \nabla \varphi(x) d\sigma_\Gamma(x) \\
& \quad - \int_\Gamma n(x) \cdot \nabla (\phi_1 - \phi_2)(x) \varphi(x) d\sigma_\Gamma(x) \\
& = \langle \nabla \cdot (j_\Gamma^0 \psi n \delta_\Gamma), \varphi \rangle - \langle j_\Gamma^1 \psi \delta_\Gamma, \varphi \rangle,
\end{aligned}$$

one has

$$S_1^* \tilde{\oplus} S_2^* \psi = -\Delta \psi + V - j_\Gamma^1 \psi \delta_\Gamma - \nabla \cdot (j_\Gamma^0 \psi n \delta_\Gamma).$$

Since  $S_1^* \tilde{\oplus} S_2^*$  is a closed operator and

$$\mathcal{D}_k(\mathbb{R}^d) := \{\psi_k = R_k \phi_k, \phi_k \in \mathcal{D}(\mathbb{R}^d)\}$$

is dense, w.r.t. the graph norm, in  $D(S_k^*) \equiv D(\Delta_{\Omega_k}^{\max})$  (see [31], Lemma 2.2, [32], Chapter 2, Section 6.4), the above additive representation of  $S_1^* \tilde{\oplus} S_2^*$  extends from  $\mathcal{D}_1(\mathbb{R}^d) \tilde{\oplus} \mathcal{D}_2(\mathbb{R}^d)$  to  $D(\Delta_{\Omega_1}^{\max}) \tilde{\oplus} D(\Delta_{\Omega_2}^{\max})$  and so one has the following

**Theorem 3.2.**

$$\begin{aligned}
& S_1^* \tilde{\oplus} S_2^* : D(\Delta_{\Omega_1}^{\max}) \tilde{\oplus} D(\Delta_{\Omega_2}^{\max}) \subseteq L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d), \\
& S_1^* \tilde{\oplus} S_2^* \psi = -\Delta \psi + V \psi - j_\Gamma^1 \psi \delta_\Gamma - \nabla \cdot (j_\Gamma^0 \psi n \delta_\Gamma).
\end{aligned}$$

We can now restrict  $S_1^* \tilde{\oplus} S_2^*$  to  $D(H_1) \tilde{\oplus} D(H_2)$  thus obtaining a self-adjoint operator  $H$  which satisfies conditions (1) to (3). In particular we can restrict  $S_1^* \tilde{\oplus} S_2^*$  to the domains corresponding to the most common local boundary conditions at the boundary of  $\Omega$ : Dirichlet, Neumann and Robin boundary conditions i.e. to

$$D(\Delta_{\Omega_1}^D) \tilde{\oplus} D(\Delta_{\Omega_2}^D), \quad D(\Delta_{\Omega_1}^N) \tilde{\oplus} D(\Delta_{\Omega_2}^N) \quad \text{and} \quad D(\Delta_{\Omega_1}^R) \tilde{\oplus} D(\Delta_{\Omega_2}^R),$$

where

$$\begin{aligned}
D(\Delta_{\Omega_k}^D) &:= \{\psi_k \in H^2(\Omega_k) : \gamma_{\Omega_k}^0 \psi_k = 0\}, \\
D(\Delta_{\Omega_k}^N) &:= \{\psi_k \in H^2(\Omega_k) : \gamma_{\Omega_k}^1 \psi_k = 0\}, \\
D(\Delta_{\Omega_k}^R) &:= \{\psi_k \in H^2(\Omega_k) : \gamma_{\Omega_k}^1 \psi_k = f_k \gamma_{\Omega_k}^0 \psi_k\},
\end{aligned}$$

$f_k \in C^\infty(\Gamma)$ ,  $f_k = f_k^*$ . We denote by  $H^D$ ,  $H^N$  and  $H^R$  the corresponding self-adjoint operators.

Now we use the representation of  $S_1^* \tilde{\oplus} S_2^*$  obtained above to recast any separating self-adjoint extension

$$H_1 \tilde{\oplus} H_2$$

in the form

$$H = -\Delta + V + B,$$

with  $H$  defined on its maximal domain.

Let

$$F_k : D(\Delta_{\Omega_k}^{\max}) \rightarrow \mathcal{D}'(\Gamma)$$

be any map such that

$$D(H_k) = \text{Ker}(F_k).$$

Then

**Theorem 3.3.**  $H_1 \tilde{\oplus} H_2 = H$ , where

$$H : D(H) \subseteq L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d), \quad H = -\Delta + V + B,$$

$$D(H) = \{\psi \in D(\Delta_{\Omega_1}^{\max}) \tilde{\oplus} D(\Delta_{\Omega_2}^{\max}) : -\Delta\psi + V\psi + B\psi \in L^2(\mathbb{R}^d)\},$$

$$B\psi = F\psi - j_\Gamma^1 \psi \delta_\Gamma - \nabla \cdot (j_\Gamma^0 \psi n \delta_\Gamma)$$

$$F\psi := c_1(F_1\psi_1 + F_2\psi_2)\delta_\Gamma + c_2 \nabla \cdot ((F_1\psi_1 - F_2\psi_2)n\delta_\Gamma), \quad c_1 c_2 \neq 0.$$

*Proof.* For any  $\psi = \psi_1 \tilde{\oplus} \psi_2 \in D(\Delta_{\Omega_1}^{\max}) \tilde{\oplus} D(\Delta_{\Omega_2}^{\max})$  one has

$$-\Delta\psi + V\psi + B\psi = S_1^* \tilde{\oplus} S_2^* \psi + F\psi$$

and so

$$-\Delta\psi + V\psi + B\psi \in L^2(\mathbb{R}^d) \iff F\psi = 0$$

$$\iff \psi_k \in \text{Ker}(F_k), \quad k = 1, 2, \iff \psi \in D(H_1 \tilde{\oplus} H_2),$$

i.e.  $D(H) = D(H_1 \tilde{\oplus} H_2)$ . The proof is then concluded by  $H \subseteq S_1^* \tilde{\oplus} S_2^*$ .  $\square$

Let us define the boundary singular potential

$$B^D : D(\Delta_{\Omega_1}^{\max}) \tilde{\oplus} D(\Delta_{\Omega_2}^{\max}) \rightarrow \mathcal{D}'(\mathbb{R}^d), \quad B^D \psi := (\mu_\Gamma^0 \psi - j_\Gamma^1 \psi) \delta_\Gamma,$$

where

$$\mu_\Gamma^0 : D(\Delta_{\Omega_1}^{\max}) \tilde{\oplus} D(\Delta_{\Omega_2}^{\max}) \rightarrow \mathcal{D}'(\Gamma), \quad \mu_\Gamma^0 \psi := \frac{1}{2} (\hat{\gamma}_{\Omega_1}^0 \psi_1 + \hat{\gamma}_{\Omega_2}^0 \psi_2),$$

is the mean of the inner and outer limits at  $\Gamma$  of  $\psi = E_1\psi_1 + E_2\psi_2$ .  
Then

**Corollary 3.4.**

$$H^D : D(H^D) \subseteq L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d), \quad H^D = -\Delta + V + B^D,$$

$$D(H^D) = \{\psi \in D(\Delta_{\Omega_1}^{\max}) \tilde{\oplus} D(\Delta_{\Omega_2}^{\max}) : -\Delta\psi + V\psi + B^D\psi \in L^2(\mathbb{R}^d)\}.$$

*Proof.* By taking  $F_k = F_k^D$ ,

$$F_k^D : D(\Delta_{\Omega_k}^{\max}) \rightarrow \mathcal{D}'(\Gamma), \quad F_k^D \psi_k := \hat{\gamma}_{\Omega_k}^0 \psi_k,$$

one has

$$D(\Delta_{\Omega_k}^D) = \text{Ker}(F_k^D)$$

by elliptic regularity. The proof is then concluded by

$$\begin{aligned} & \frac{1}{2} (F_1^D \psi_1 + F_2^D \psi_2) \delta_\Gamma + \nabla \cdot ((F_1^D \psi_1 - F_2^D \psi_2) n \delta_\Gamma) \\ & - j_\Gamma^1 \psi \delta_\Gamma - \nabla \cdot (j_\Gamma^0 \psi n \delta_\Gamma) \\ & = B^D \psi. \end{aligned}$$

□

A similar result can be obtained in the case of Neumann boundary conditions. In this case we define the boundary singular potential

$$B^N : D(\Delta_{\Omega_1}^{\max}) \tilde{\oplus} D(\Delta_{\Omega_2}^{\max}) \rightarrow \mathcal{D}'(\mathbb{R}^d), \quad B^N \psi := \nabla \cdot ((\mu_\Gamma^1 \psi - j_\Gamma^0 \psi) n \delta_\Gamma),$$

where

$$\mu_\Gamma^1 : D(\Delta_{\Omega_1}^{\max}) \tilde{\oplus} D(\Delta_{\Omega_2}^{\max}) \rightarrow \mathcal{D}'(\Gamma), \quad \mu_\Gamma^1 \psi := \frac{1}{2} (\hat{\gamma}_{\Omega_1}^1 \psi_1 - \hat{\gamma}_{\Omega_2}^1 \psi_2),$$

is the mean of the inner and outer limits at  $\Gamma$  of the normal derivative of  $\psi = E_1 \psi_1 + E_2 \psi_2$ . Then

**Corollary 3.5.**

$$H^N : D(H^N) \subseteq L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d), \quad H^N = -\Delta + V + B^N,$$

$$D(H^N) = \{\psi \in D(\Delta_{\Omega_1}^{\max}) \tilde{\oplus} D(\Delta_{\Omega_2}^{\max}) : -\Delta \psi + V \psi + B^N \psi \in L^2(\mathbb{R}^d)\}.$$

*Proof.* By taking  $F_k = F_k^N$ ,

$$F_k^N : D(\Delta_{\Omega_k}^{\max}) \rightarrow \mathcal{D}'(\Gamma), \quad F_k^N \psi_k := \hat{\gamma}_{\Omega_k}^1 \psi_k,$$

one has

$$D(\Delta_{\Omega_k}^N) = \text{Ker}(F_k^N)$$

by elliptic regularity. The proof is then concluded by

$$\begin{aligned} & (F_1^N \psi_1 + F_2^N \psi_2) \delta_\Gamma + \frac{1}{2} \nabla \cdot ((F_1^N \psi_1 - F_2^N \psi_2) n \delta_\Gamma) \\ & - j_\Gamma^1 \psi \delta_\Gamma - \nabla \cdot (j_\Gamma^0 \psi n \delta_\Gamma) \\ & = B^N \psi. \end{aligned}$$

□

The case of Robin boundary conditions is no more than a combination of the two preceding ones by taking

$$F_k = F_k^R := F_k^N - f_k F_k^D.$$

So, by defining

$$B^R : D(\Delta_{\Omega_1}^{\max}) \tilde{\oplus} D(\Delta_{\Omega_2}^{\max}) \rightarrow \mathcal{D}'(\mathbb{R}^d),$$

$$B^R \psi := \nabla \cdot ((\mu_\Gamma^1 \psi - \mu_\Gamma^{0,f_1,f_2} \psi - j_\Gamma^0 \psi) n \delta_\Gamma) - j_\Gamma^{0,f_1,f_2} \psi \delta_\Gamma,$$

where

$$\mu_\Gamma^{0,f_1,f_2} : D(\Delta_{\Omega_1}^{\max}) \tilde{\oplus} D(\Delta_{\Omega_2}^{\max}) \rightarrow \mathcal{D}'(\mathbb{R}^d), \quad \mu_\Gamma^{0,f_1,f_2} \psi := \frac{1}{2} (f_1 \hat{\gamma}_{\Omega_1}^0 \psi_1 - f_2 \hat{\gamma}_{\Omega_2}^0 \psi_2),$$

$$j_\Gamma^{0,f_1,f_2} : D(\Delta_{\Omega_1}^{\max}) \tilde{\oplus} D(\Delta_{\Omega_2}^{\max}) \rightarrow \mathcal{D}'(\Gamma), \quad j_\Gamma^{0,f_1,f_2} \psi := f_1 \hat{\gamma}_{\Omega_1}^0 \psi_1 + f_2 \hat{\gamma}_{\Omega_2}^0 \psi_2,$$

one has

**Corollary 3.6.**

$$H^R : D(H^R) \subset L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d), \quad H^R = -\Delta + V + B^R,$$

$$D(H^R) = \{\psi \in D(\Delta_{\Omega_1}^{\max}) \tilde{\oplus} D(\Delta_{\Omega_2}^{\max}) : -\Delta \psi + V \psi + B^R \psi \in L^2(\mathbb{R}^d)\}.$$

We conclude by discussing the case of a general (non-local) boundary conditions.

The most general separating self-adjoint extension are of the kind  $H_1 \tilde{\oplus} H_2$ , with (see [24, 40, 41, 25] and references therein)

$$H_k : D(H_k) \subseteq L^2(\Omega_k) \rightarrow L^2(\Omega_k), \quad H_k \psi_k := -\Delta_{\Omega_k} \psi_k + V_k \psi_k,$$

$$D(H_k) = \{\psi_k \in D(\Delta_{\Omega_k}^{\max}) : \Sigma \hat{\gamma}_{\Omega_k}^0 \psi_k \in D(\Theta_k),$$

$$\Pi_k(\hat{\gamma}_{\Omega_k}^1 \psi_k - P_{\Omega_k}^{DN} \hat{\gamma}_{\Omega_k}^0 \psi_k) = \Theta_k \Sigma \hat{\gamma}_{\Omega_k}^0 \psi_k\},$$

where  $\Pi_k$  is an orthogonal projector in  $H^{1/2}(\Gamma)$ ,  $\Sigma$  is the canonical unitary isomorphism mapping the space  $H^s(\Gamma)$  onto  $H^{s+1}(\Gamma)$ ,  $\Theta_k$  is a self-adjoint operator acting in the Hilbert space given by the the range of  $\Pi_k$ ,  $P_{\Omega_k}^{DN} : H^s(\Gamma) \rightarrow H^{s-1}(\Gamma)$  is the Dirichlet-to-Neumann operator (relative to  $\Omega_k$ ) over  $\Gamma$ . Let us remark that for any  $\psi_k \in D(\Delta_{\Omega_k}^{\max})$  the difference  $\hat{\gamma}_{\Omega_k}^1 \psi_k - P_{\Omega_k}^{DN} \hat{\gamma}_{\Omega_k}^0 \psi_k$  is always  $H^{1/2}(\Gamma)$ -valued.

Note that Dirichlet boundary conditions correspond to  $\Pi_k = 0$  and Robin boundary conditions correspond to  $\Pi_k = 1$  and  $\Theta_k = \Theta_k^R$ ,

$$\Theta_k^R := (-P_{\Omega_k}^{DN} + M_k) \Sigma^{-1} : H^{5/2}(\Gamma) \subset H^{1/2}(\Gamma) \rightarrow H^{1/2}(\Gamma),$$

where  $M_k$  denotes the multiplication by  $f_k$ .

For general boundary conditions one is lead to take  $F_k = \hat{F}_k$ , where

$$\hat{F}_k \psi_k := \hat{\gamma}_{\Omega_k}^0 \psi_k - \Sigma^{-1}(\Theta_k + i)^{-1} \Pi_k(\hat{\gamma}_{\Omega_k}^1 \psi_k - P_{\Omega_k}^{DN} \hat{\gamma}_{\Omega_k}^0 \psi_k - i \Sigma \hat{\gamma}_{\Omega_k}^0 \psi_k).$$

This gives  $\hat{F}_k = F_k^D$  when  $\Pi_k = 0$ , but produces

$$\hat{F}_k \psi_k = \Sigma^{-1}(\Theta_k^R + i)^{-1}(f_k \hat{\gamma}_{\Omega_k}^0 \psi_k - \hat{\gamma}_{\Omega_k}^1 \psi_k) \neq F_k^R$$

in the case of Robin boundary conditions. This shows that there exist different confining potentials for the same boundary conditions, some being more convenient than others.

**Remark 3.7.** Is it possible to use alternative (i.e. which use different extension parameters) representations of  $D(H_k)$ , as suggested by boundary triple theory (see e.g. [23] and references therein). This produces similar results. For example one can write

$$\begin{aligned} D(H_k) &= \{\psi_k \in D(\Delta_{\Omega_k}^{\max}) : i(1 + U_k)\Sigma \hat{\gamma}_{\Omega_k}^0 \psi_k \\ &= (1 - U_k)(\hat{\gamma}_{\Omega_k}^1 \psi_k - P_{\Omega_k}^{DN} \hat{\gamma}_{\Omega_k}^0 \psi_k)\}, \end{aligned}$$

where

$$U_k : H^{1/2}(\Gamma) \rightarrow H^{1/2}(\Gamma)$$

is unitary. In this case Dirichlet boundary conditions correspond to the choice  $U_k = 1$  and Robin ones to  $U_k = (\Theta_k^R - i)(\Theta_k^R + i)^{-1}$ , i.e.  $U_k$  is the Cayley transform of  $\Theta_k^R$ .

#### ACKNOWLEDGMENTS

N.C.D. and J.N.P. thank P. Garbaczewski for several discussions. N.C.D. and J.N.P. were partially supported by grant PTDC/MAT/69635/2006 of the Portuguese Science Foundation.

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